10/698,118

(FILE 'HOME' ENTERED AT 16:48:56 ON 27 NOV 2004)

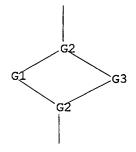
FILE 'REGISTRY' ENTERED AT 16:49:13 ON 27 NOV 2004 STRUCTURE UPLOADED

=> d 11

L1

L1 HAS NO ANSWERS

L1 STR



G1 Ag, Au, Cu

G2 O, S, Se, Te

G3 Al, Ga, In

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 16:49:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 55 TO ITERATE

100.0% PROCESSED 55 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 656 TO 1544
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:49:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 966 TO ITERATE

100.0% PROCESSED 966 ITERATIONS 38 ANSWERS

SEARCH TIME: 00.00.01

L3 38 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 155.42 155.63

FILE 'CAPLUS' ENTERED AT 16:49:43 ON 27 NOV 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 27 Nov 2004 VOL 141 ISS 23 FILE LAST UPDATED: 26 Nov 2004 (20041126/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 28 L3

=> d 1-28 bib abs

- L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2004:343960 CAPLUS
- DN 141:306353
- TI Synthesis and characterization of CuInS2 single source precursors for chemical vapor deposition
- AU Cowen, J. E.; Riga, A. T.; Hepp, A. F.; Duraj, S. A.; Banger, K.; McClarnon, R.
- CS Cleveland State University, Cleveland, OH, 44115, USA
- SO Journal of Thermal Analysis and Calorimetry (2004), 75(3), 929-936 CODEN: JTACF7; ISSN: 1388-6150
- PB Kluwer Academic Publishers
- DT Journal
- LA English
- AB A family of single source precursors, for the spray CVD of chalcopyrite thin films (CuInS2), was synthesized in good yields (.apprx.65%). Newly synthesized compds. include [{L}2Cu(SR)2In(SR)2] (R = alkyl, aryl; L = phosphine/arsine/stibine neutral donor ligand). The use of the single source precursors provides an attractive alternative over conventionally used multi-source precursors, which are often toxic, air sensitive and pyrophoric. However, it is desirable that these thin films be processed on flexible polymer substrates such as Kapton. Therefore, milder deposition temps. are needed to maintain the structural integrity of the underlying polymer substrates. By selective manipulation of the steric and electronic properties of the precursor, milder processing temps. may be employed, while maintaining the desired stoichiometry of the deposited films. Elucidation of the structures were confirmed using NMR. Thermal anal. techniques, DSC and TGA (TG), were employed to determine thermal profiles of each candidate compound
- RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2004:277396 CAPLUS
- DN 141:192917
- TI Synthesis and characterization of the first liquid single source precursors for the deposition of ternary chalcopyrite (CuInS2) thin film materials
- AU Banger, Kulbinder K.; Cowen, Jonathan; Hepp, Aloysius F.

- CS Ohio Aerospace Institute, Brook Park, OH, 44142, USA
- SO NASA/TM (2002), NASA/TM-2002-211128, 1-42 CODEN: NATMA4; ISSN: 0499-9320
- DT Report
- LA English
- OS CASREACT 141:192917
- AB Mol. engineering of ternary single source precursors based on the [{PBu3}2Cu(SR')2In(SR')2] architecture have afforded the 1st liquid CIS ternary single source precursors (when R = Et, Pr), which are suitable for low temperature deposition, (< 350°C). Thermogravimetric analyses (TGA) and Modulated-DSC confirm their liquid phase and reduced stability. X-ray diffraction studies, EDS and SEM support the formation of the single-phase chalcopyrite CuInS2 at low temps.
- RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2004:46634 CAPLUS
- DN 140:342013
- TI Chemical vapor deposition for ultra-lightweight thin-film solar arrays for space
- AU Hepp, Aloysius F.; Raffaelle, Ryne P.; Banger, Kulbinder K.; Jin, Michael H.; Lau, Janice E.; Harris, Jerry D.; Cowen, Jonathan E.; Duraj, Stan A.
- CS National Aeronautics and Space Administration, Glenn Research Center, Cleveland, OH, 44135, USA
- SO NASA/TM (2002), NASA/TM-2002-2111835, 1-6 CODEN: NATMA4; ISSN: 0499-9320
- DT Report
- LA English
- The development of thin-film solar cells on flexible, lightwt., space-qualified substrates provides an attractive cost solution to fabricating solar arrays with high sp. power (W/kg). The use of a polycryst. chalcopyrite absorber layer for thin-film solar cells is considered for the next generation photovoltaic devices. This creates a need for low-cost high-throughput manufacturing of high-efficiency thin-film solar cells. New single-source-precursors (SSP's) and their use in deposition of chalcopyrite semi-conducting layers (CIS) onto flexible substrates for solar cell fabrication are discussed. The syntheses and thermal modulation of SSP's via mol. engineering is described. Thin-film fabrication studies demonstrate that the SSPs can be used in a spray CVD process for depositing CIS at reduced temps., which has good elec. properties suitable for PV devices.
- RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:860654 CAPLUS
- DN 140:67846
- TI A New Facile Route for the Preparation of Single-Source Precursors for Bulk, Thin-Film, and Nanocrystallite I-III-VI Semiconductors
- AU Banger, Kulbinder K.; Jin, Michael H.-C.; Harris, Jerry D.; Fanwick, Philip E.; Hepp, Aloysius F.
- CS Ohio Aerospace Institute, Cleveland, OH, 44142, USA
- SO Inorganic Chemistry (2003), 42(24), 7713-7715 CODEN: INOCAJ; ISSN: 0020-1669
- PB American Chemical Society
- DT Journal
- LA English
- AB The authors report a new simplified synthetic procedure for com. manufacture of ternary single-source precursors (SSPs). This new synthetic process was successfully implemented to fabricate known SSPs on bulk scale and the 1st liquid SSPs to the semiconductors CuInSe2 and AgInxSy. Single crystal x-ray

determination reveals the 1st unsolvated ternary AgInS SSP. SSPs prepared via this

new route have successfully been used in a spray assisted CVD process to deposit polycryst. thin films, and for preparing ternary nanocrystallites.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:822014 CAPLUS
- DN 140:50503
- TI The effect of film composition on the texture and grain size of CuInS2 prepared by chemical spray pyrolysis
- AU Jin, Michael H.-C.; Banger, Kulbinder K.; Harris, Jerry D.; Hepp, Aloysius
- CS Ohio Aerospace Institute, Brookpark, OH, 44142, USA
- SO Materials Research Society Symposium Proceedings (2003), 763 (Compound Semiconductor Photovoltaics), 403-408 CODEN: MRSPDH; ISSN: 0272-9172
- PB Materials Research Society
- DT Journal
- LA English
- Ternary single-source precursors were used to deposit CuInS2 thin films AΒ using chemical spray pyrolysis. The authors studied the effect of the film composition on texture, secondary phase formation, and grain size. either (112) - or (204/220) - preferred orientation were deposited with most often In-rich composition The (112)-preferred orientation became more pronounced as the film composition became more In-poor. Films with a (204/220)-preferred orientation were both In-rich and contained a yet unidentified secondary phase. The phase was evaluated as an In-rich compound based on composition anal. and Raman spectroscopy. Further the phase could be removed by depositing a thin Cu layer prior to the growth of CuInS2. Similarly, as-grown Cu-rich (112)-oriented films did not exhibit the In-rich compound The (204/220) preferred orientation of the film is likely related to the equivalent symmetry between planes of CuInS2 and the In-rich compound The largest grain size (.apprx. 0.5 µm) was achieved with Cu-rich (112)-oriented films.
- RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:491570 CAPLUS
- DN 139:189925
- TI Nanocrystalline Chalcopyrite Materials (CuInS2 and CuInSe2) via Low-Temperature Pyrolysis of Molecular Single-Source Precursors
- AU Castro, Stephanie L.; Bailey, Sheila G.; Raffaelle, Ryne P.; Banger, Kulbinder K.; Hepp, Aloysius F.
- CS Ohio Aerospace Institute, Cleveland, OH, 44142, USA
- SO Chemistry of Materials (2003), 15(16), 3142-3147 CODEN: CMATEX; ISSN: 0897-4756
- PB American Chemical Society
- DT Journal
- LA English
- Nanometer-sized particles of the chalcopyrite compds. CuInS2 and CuInSe2 were synthesized by thermal decomposition of mol. single-source precursors (PPh3)2CuIn(SEt)4 and (PPh3)2CuIn(SePh)4, resp., in the noncoordinating solvent dioctyl phthalate at 200-300°. The nanoparticles range in size from 3 to 30 nm and are aggregated to form roughly spherical clusters of .apprx.500 nm in diameter X-ray diffraction of the nanoparticle powders shows greatly broadened lines, indicative of very small particle sizes, which is confirmed by TEM. Peaks present in the XRD can be indexed to reference patterns for the resp. chalcopyrite compds. Optical spectroscopy and elemental anal. by energy dispersive spectroscopy support the

identification of the nanoparticles as chalcopyrites.

RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:428255 CAPLUS
- DN 139:294436
- TI Single source precursors for fabrication of I-III-VI2 thin-film solar cells via spray CVD
- AU Hollingsworth, J. A.; Banger, K. K.; Jin, M. H.-C.; Harris, J. D.; Cowen, J. E.; Bohannan, E. W.; Switzer, J. A.; Buhro, W. E.; Hepp, A. F.
- CS Department of Chemistry, Washington University, St. Louis, MO, 63130, USA
- SO Thin Solid Films (2003), 431-432, 63-67 CODEN: THSFAP; ISSN: 0040-6090
- PB Elsevier Science B.V.
- DT Journal
- LA English
- The development of thin-film solar cells on flexible, lightwt., space-qualified substrates provides an attractive cost solution to fabricating solar arrays with high sp. power (W/kg). Thin-film fabrication studies demonstrate that ternary single source precursors can be used in either a hot or cold-wall spray chemical vapor deposition (CVD) reactor for depositing CuInS2, CuGaS2, and Cu(Ga,In)S2 at reduced temps. (400-450°), which display good elec. and optical properties suitable for photovoltaic devices. X-ray diffraction studies, energy dispersive spectroscopy, and SEM confirmed the formation of the single-phase CuInS2, CuGaS2, and Cu(Ga,In)S2 thin films on various substrates at reduced temps.
- RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:383457 CAPLUS
- DN 139:309891
- TI A review of single source precursors for the deposition of ternary chalcopyrite materials
- AU Banger, K. K.; Cowen, J.; Harris, J.; McClarnon, R.; Hehemann, D. G.; Duraj, S. A.; Scheiman, D.; Hepp, A. F.
- CS Ohio Aerospace Institute, Brookpark, OH, 44142, USA
- NASA Conference Publication (2002), 2002-211831(17th Space Photovoltaic Research and Technology Conference, 2001), 115-125 CODEN: NACPDX; ISSN: 0191-7811
- PB National Aeronautics and Space Administration
- DT Journal; (computer optical disk)
- LA English
- The development of thin-film solar cells on flexible, lightwt., AΒ space-qualified durable substrates (i.e. Kapton) provides an attractive solution to fabricating solar arrays with high sp. power. The syntheses and thermal modulation of ternary single source precursors, based on the [{LR}2Cu(SR')2In(SR')2]-architecture, in good yields, are described. TGA and low-temperature DSC demonstrate that controlled manipulation of the steric and electronic properties of either the group 5-donor and/or chalcogenide moiety permits directed adjustment of the thermal stability and phys. properties of the precursors. TGA-Evolved Gas Anal., confirms that single precursors decompose by the initial expulsion of the sulfide moiety, followed by the loss of the neutral donor group, (L) to release the ternary chalcopyrite matrix. XRD studies, EDS and SEM of the nonvolatile pyrolyzed material demonstrate that these derivs. produce single-phase CuInS2/CuInSe2 materials at low temperature Thin-film fabrication studies demonstrate that these single source precursors can be used in a spray CVD process to deposit CuInS2 onto flexible polymer substrates at temps. <400°.

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:383454 CAPLUS
- DN 139:152228
- TI Atmospheric pressure spray chemical vapor deposited CuInS2 thin films for photovoltaic applications
- AU Harris, J. D.; Raffaelle, R. P.; Banger, K. K.; Smith, M. A.; Scheiman, D. A.; Hepp, A. F.
- CS Cleveland State University, Cleveland, OH, 44115, USA
- NASA Conference Publication (2002), 2002-211831(17th Space Photovoltaic Research and Technology Conference, 2001), 84-90 CODEN: NACPDX; ISSN: 0191-7811
- PB National Aeronautics and Space Administration
- DT Journal; (computer optical disk)
- LA English
- AB Solar cells have been prepared using atmospheric pressure spray chemical vapor deposited CuInS2 absorbers. The CuInS2 films were deposited at 390° using single source precursor (PPh3)2CuIn(SEt)4 in an argon atmospheric The absorber ranges in thickness from 0.75 to 1.0 μm, and exhibits a crystallog. gradient, with the leading edge having a (220) preferred orientation and the trailing edge having a (112) orientation. Schottky diodes prepared by thermal evaporation of aluminum contacts on to the CuInS2 yielded diodes for films that were annealed at 600°. Solar cells were prepared using annealed films and had the (top-to-down) composition

of
Al/ZnO/CdS/CuInS2/Mo/glass. The short-circuit current, open-circuit
voltage, fill factor, and efficiency were 6.46 mA/cm2, 307 mV, 24%, and
0.35%, resp., for the best small area cells under simulated air-mass 0
illumination.

- RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:365416 CAPLUS
- DN 139:94254
- TI Novel Bimetallic Thiocarboxylate Compounds as Single-Source Precursors to Binary and Ternary Metal Sulfide Materials
- AU Deivaraj, Theivanayagam C.; Park, Jin-Ho; Afzaal, Mohammad; O'Brien, Paul; Vittal, Jagadese J.
- CS Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore
- SO Chemistry of Materials (2003), 15(12), 2383-2391 CODEN: CMATEX; ISSN: 0897-4756
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 139:94254
- Binuclear [(Ph3P)CuM(SC(O)Ph)4] (M = Ga (1) or In (2)),
 [(Ph3P)2AgGa(SC(O)Ph)4] (3), [(Ph3P)2AgIn(SC(O)R)4] (R = Me (4) or Ph (5))
 were synthesized and characterized. The solid-state structures of compds.
 1-3 were determined by x-ray crystallog. TG and pyrolysis studies revealed
 that these compds. decompose to give the corresponding ternary metal sulfide
 materials. However, using the aerosol-assisted CVD (AACVD) method, In2S3
 thin films were obtained from 2 and AgIn5S8 thin films were obtained from
 compds. 4 and 5.
- RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:315506 CAPLUS

- DN 139:119828
- TI Characterization of CuInS2 films prepared by atmospheric pressure spray chemical vapor deposition
- AU Harris, Jerry D.; Banger, Kulbinder K.; Scheiman, David A.; Smith, Mark A.; Jin, Michael H.-C.; Hepp, Aloysius F.
- CS Department of Chemistry, Cleveland State University, Cleveland, OH, 44115, USA
- SO Materials Science & Engineering; B: Solid-State Materials for Advanced Technology (2003), B98(2), 150-155 CODEN: MSBTEK; ISSN: 0921-5107
- PB Elsevier Science B.V.
- DT Journal
- LA English
- AB CuInS2 films were deposited by atmospheric pressure spray CVD. Films were deposited at 390° using [(PPh3)2CuIn(SEt)4] as a single source precursor in an Ar atmospheric The films range in thickness from 0.75 to 1.0 µm and exhibit a crystallog. gradient, with the leading edge having a (220) preferred orientation and the trailing edge having a (112) orientation. Schottky diodes prepared by thermal evaporation of Al contacts

the CuInS2 yielded diodes for films that were annealed at 600°. The photoresponse of several films was measured by photoelectrochem. anal. in an aqueous, acidic electrolyte. Prolonged exposure of the films to the electrolyte decreased the photoresponse. Complete solar cells were prepared using annealed films with a (top down) composition of Al/ZnO/CdS/CuInS2/Mo/Glass. The values for the short-circuit current, open-circuit voltage, maximum power output (Pmax), current at Pmax (Imax), voltage at Pmax (Vmax), fill factor and efficiency were 5.25 mA, 304 mV, 0.470 mW, 2.92 mA, 161 mV, 29.4 and 0.68%, resp., for a 0.5 cm2 cell under simulated AMO illumination.

- RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2003:243913 CAPLUS
- DN 139:94219
- TI Synthesis, characterization, and spectroscopic properties of heterobimetallic isopropoxides of Co, Ni and Cu containing diethanolaminate moiety
- AU Sharma, Kanupriya; Sharma, Malti; Singh, Anirudh; Mehrotra, Ram C.
- CS Department of Chemistry, University of Rajasthan, Jaipur, 302 004, India
- SO Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (2003), 42A(3), 493-498 CODEN: ICACEC; ISSN: 0376-4710
- PB National Institute of Science Communication
- DT Journal
- LA English
- OS CASREACT 139:94219
- AB Hydrocarbon-insol. derivs. M(deaH)2 (M = Co, Ni, Cu; deaH2 = diethanolamine) on reactions with Al(OPri)3 in 1:2 molar ratio yield hydrocarbon-soluble, monomeric heterobimetallic derivs.

 [{Al(OPri)2}2M(dea)2]. A different type of soluble heteroleptic derivs. was prepared by the reactions of M{Al(OPri)4}2 with deaH2 in 1:1, 1:2 and 1:3 molar ratios. The reaction of M{Al(OPri)4}2 with four equivalent of diethanolamine yields a benzene insol. product M{Al(dea)2}2. All these new derivs. were characterized by elemental analyses, mol. weight measurements and spectroscopic (Electronic and IR) studies.
- RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN AN 2002:974910 CAPLUS

- DN 138:306675
- TI Single-source approach for the growth of I-III-VI thin films
- AU Afzaal, Mohammad; Deivaraj, Theivanayagam C.; O'Brien, Paul; Park, Jin-Ho; Vittal, Jagadese J.
- CS The Manchester Materials Science Centre and Department of Chemistry, University of Manchester, Manchester, M13 9PL, UK
- SO Materials Research Society Symposium Proceedings (2002), 730 (Materials for Energy Storage, Generation and Transport), 185-190 CODEN: MRSPDH; ISSN: 0272-9172
- PB Materials Research Society
- DT Journal
- LA English
- AB The ternary chalcopyrite semiconductors, I-III-VI, are currently used for photovoltaic solar cell applications. AgIn5S8 thin films were prepared from single-source bimetalorg. precursors [e.g. (PPh3)2AgIn(SC{0}R)4, R = alkyl] by aerosol assisted CVD (AA-CVD). These compds. can be used as single-source precursors for the deposition of the ternary cholcopyrite semiconductors by one-pot reactions using the AA-CVD process. In addition, these compds. are air stable, which is favorable in comparison with metal alkyl compds. which are pyrophoric. The optimum growth temperature for the preparation of these films on glass and on Si(100) substrates is >350° in terms of crystallinity, although deposition occurred at low temps. The films were studied using XRD, SEM and EDS. SEM anal. shows that all films are microcryst. but have different morphologies depending on the growth temps. XRD results show evidence of the crystalline nature of these films. Results are presented and discussed.
- RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2002:378096 CAPLUS
- DN 137:102977
- TI Extending the Coordination Chemistry of Molecular P4S3: The Polymeric Ag(P4S3) + and Ag(P4S3)2+ Cations
- AU Adolf, Ariane; Gonsior, Marcin; Krossing, Ingo
- CS Institut fuer Anorganische Chemie, Universitaet Karlsruhe, Karlsruhe, D-76128, Germany
- SO Journal of the American Chemical Society (2002), 124(24), 7111-7116 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- Upon reacting P4S3 with AgAl(hfip)4 and AgAl(pftb)4 [hfip = OC(H)(CF3)2; AΒ pftb = OC(CF3)3, the compds. Ag(P4S3)Al(hfip)4 (1) and Ag(P4S3)2+[Al(pftb)4]- (2) formed in CS2 or CS2/CH2Cl2 solution, resp. Compds. 1 and 2 were characterized by single-crystal x-ray structure detns., Raman and solution NMR spectroscopy, and elemental analyses. One-dimensional chains of $[Ag(P4S3)x] \infty$ (x = 1 (1); x = 2 (2)) formed in the solid state with P4S3 ligands that bridge through a 1,3-P,S, a 2,4-P,S, or a 3,4-P,P η 1 coordination to the silver ions. Compound 2 with the least basic anion contains the 1st homoleptic metal (P4S3) complex. Compds. 1 and 2 also include the long sought sulfur coordination of P4S3. Raman spectra of 1 and 2 were assigned from DFT calcns. of related species. The influence of the silver coordination on the geometry of the P4S3 cage is discussed, addnl. aided by DFT calcns. Consequences for the frequently observed degradation of the cage are suggested. An exptl. silver ion affinity scale based on the solid-state structures of several weak Lewis acid base adducts (L) AgAl (hfip) 4 is given. The affinity of the ligand L to the silver ion increases according to P4 < CH2Cl2 < P4S3 < S8 < 1,2-C2H4Cl2 < toluene.
- RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2002:140318 CAPLUS
- DN 136:349702
- TI Superweak complexes of tetrahedral P4 molecules with the silver cation of weakly coordinating anions
- AU Krossing, Ingo; Van Wullen, Leo
- CS Institut fur Anorganische Chemie, Universitat Karlsruhe, Karlsruhe, 76128, Germany
- SO Chemistry--A European Journal (2002), 8(3), 700-711 CODEN: CEUJED; ISSN: 0947-6539
- PB Wiley-VCH Verlag GmbH
- DT Journal
- LA English
- OS CASREACT 136:349702
- The silver aluminates AgAl[OC(CF3)2(R)]4 (R = H, CH3, CF3) react with AΒ solns. of white phosphorus P4 to give complexes that bind one or two almost undistorted tetrahedral P4 mols. in an $\eta 2$ fashion: [Ag(P4)2]+[Al(OC(CF3)3)4]-(1) containing the 1st homoleptic metal-phosphorus cation, the mol. species (P4)AgAl[OCMe(CF3)2]4 (2), and the dimeric Ag(μ , η 2-P4)Ag bridged {(P4)AgAl[OC(H)(CF3)2]4}2 (3). Compds. 1-3 were characterized by variable-temperature (VT) 31P NMR spectroscopy (1 also by VT 31P MAS NMR spectroscopy), Raman spectroscopy, and single-crystal x-ray crystallog. Other Ag:P4 ratios did not lead to new species, and this observation was rationalized on thermodn. grounds. The Ag(P4)2+ ion has an almost planar coordination environment around the Ag+ ion due to $dx2-y2(Ag) \rightarrow \sigma^*(P-P)$ backbonding. Calcns. (HF-DFT) on six $Aq(P_4)2+$ isomers showed that the planar η^2 form is only slightly favored by 5.2 kJ mol-1 over the tetrahedral η2 species; η1-P4 and n3-P4 complexes are less favorable (27-76 kJ mol-1). The bonding of the P4 moiety in [RhCl(η 2-P4)(PPh3)2], the only compound in which an $\eta 2$ bonding mode of a tetrahedral P4 mol. was claimed, must be regarded as a tetraphosphabicyclobutane, and not as a tetrahedro-P4 complex, from the published NMR and vibrational spectra, the calculated geometry of [RhCl(P4)(PH3)2] (10), the highly endothermic (385 kJ mol-1) calculated dissociation enthalpy of 10 into P4 and RhCl(PH3)2 (11), as well as atoms in mols. (AIM) and natural bond orbital (NBO) population analyses of 10 and the Ag(P4)2+ ion. Therefore, 1-3 are the 1st examples of species containing n2-coordinated tetrahedral P4 mols.
- RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2002:81783 CAPLUS
- DN 137:65628
- TI Facile modulation of single source precursors: the synthesis and characterization of single source precursors for deposition of ternary chalcopyrite materials
- AU Banger, K. K.; Harris, J. D.; Cowen, J. E.; Hepp, A. F.
- CS Thin Film Technology Group, NASA Glenn Research Center, Cleveland, OH, 44135, USA
- SO Thin Solid Films (2002), 403-404, 390-395 CODEN: THSFAP; ISSN: 0040-6090
- PB Elsevier Science S.A.
- DT Journal
- LA English
- The syntheses and controlled thermal decomposition of ternary single-source-precursors for preparation of copper indium disulfide (CuInS2) thin films was studied, using precursors of structure (ER3)2Cu(YR')2In(YR')2 (I; E = P, As, Sb; Y = S, Se; and R = alkyl, aryl). Good yields of thin-film CuInS2 were obtained for I (R = Bu, Y = S; and R' = Et or Pr) on flexible polymeric substrates at <400°. These new

compds. were decomposed by spray chemical vapor deposition to CuInS2, an absorber layer for the fabrication of thin-film solar cells. Thermogravimetric analyses (TGA) and differential scanning calorimetry demonstrated that controlled manipulation of the steric and electronic properties of either the Group V donor and/or chalcogenide moiety resulted in a directed adjustment of the thermal stability and phys. properties of the precursor. Preliminary studies showed that these compds. produced single-phase CuInS2 thin films at low temperature, which was confirmed by x-ray diffraction, energy dispersive spectrometry, and SEM.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
```

AN 2001:826008 CAPLUS

DN 136:193190

TI Single-source precursors to ternary silver indium sulfide materials

- AU Deivaraj, Theivanayagam C.; Park, Jin-Ho; Afzaal, Mohammmad; O'Brien, Paul; Vittal, Jagadese J.
- CS Department of Chemistry, National University of, Singapore
- SO Chemical Communications (Cambridge, United Kingdom) (2001), (22), 2304-2305

CODEN: CHCOFS; ISSN: 1359-7345

- PB Royal Society of Chemistry
- DT Journal
- LA English
- OS CASREACT 136:193190
- AB [(Ph3P)2AgIn(SC{0}R)4] (R = Me, Ph) were prepared, characterized,, and used as excellent single-source precursors for AgInS2 bulk materials by pyrolysis and AgIn5S8 films by aerosol assisted CVD (AACVD). Crystals of the chloroform solvate of the Ph complex are triclinic, space group P.hivin.1, with a 12.7284(5), b 14.3145(6), c 18.7071(7) Å, α 90.716(1), β 99.624(1), γ 110.728(1)°; Z = 2, dc = 1.500; R = 0.0486, Rw = 0.0802.
- RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2001:792600 CAPLUS
- DN 136:95012
- TI Synthesis and Characterization of the First Liquid Single-Source Precursors for the Deposition of Ternary Chalcopyrite (CuInS2) Thin Film Materials
- AU Banger, Kulbinder K.; Cowen, Jonathan; Hepp, Aloysius F.
- CS Ohio Aerospace Institute, Cleveland, OH, 44142, USA
- SO Chemistry of Materials (2001), 13(11), 3827-3829 CODEN: CMATEX; ISSN: 0897-4756
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 136:95012
- AB Mol. engineering of ternary single-source precursors based on the [(PBu3)2Cu(SR)2In(SR)2] architecture have afforded the first liquid CIS ternary single-source precursors (when R = Et, n-Pr), which are suitable for low-temperature deposition (<350°). Thermogravimetric analyses (TGA) and modulated DSC confirm their liquid phase and reduced stability. X-ray diffraction studies, EDS, and SEM support the formation of the single-phase chalcopyrite CuInS2 at low temps.
- RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2001:381747 CAPLUS

- DN 135:155059
- Using single source precursors and spray chemical vapor deposition to grow ΤI thin-film CuInS2
- Harris, Jerry D.; Hehemann, David G.; Cowen, Jonathan E.; Hepp, Aloysius ΑU F.; Raffaelle, Ryne P.; Hollingsworth, Jennifer A.
- School of Technology, Kent State University, Kent, OH, 44242, USA CS
- Conference Record of the IEEE Photovoltaic Specialists Conference (2000), SO 28th, 563-566

CODEN: CRCNDP; ISSN: 0160-8371

- PB Institute of Electrical and Electronics Engineers
- DT Journal
- LA English
- Thin films of CuInS2 were deposited on fused silica, stainless steel, AΒ Kapton and polybenzobisoxazole using the single source organometallic precursor (PPh3)2CuIn(SEt)4, in conjunction with spray chemical vapor deposition. Films were deposited at temps. ranging from 325 -360°C. As deposited, the films had a thickness on the order of 200 A. The grain structure of the films was found to vary with carrier gas flow rate and substrate temperature
- THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 9 ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4ANSWER 20 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1999:407704 CAPLUS
- DN 131:80925
- TI Spray CVD of copper indium disulfide films. Control of microstructure and crystallographic orientation
- AU Hollingsworth, Jennifer A.; Hepp, Aloysius F.; Buhro, William E.
- CS Dep. Chem., Washington Univ., St. Louis, MO, 63130, USA
- SO Chemical Vapor Deposition (1999), 5(3), 105-108 Published in: Adv. Mater. (Weinheim, Ger.), 11(8) CODEN: CVDEFX; ISSN: 0948-1907
- PB Wiley-VCH Verlag GmbH
- DT Journal
- LΑ English
- The deposition of dense crystalline CuInS2 films by spray CVD from a single AB source precursor was investigated. Toluene solns. of the precursor (Ph3P) 2-Cu(μ-SEt2) In (SEt) 2 were employed and depositions were conducted using a warm-zone temperature of 140 \pm 10 $^{\circ}$ at substrate temps. of 405 ± 5° with Ar carrier-gas flow rates of 2.7-5.3 L/min. Wavelength-dispersive x-ray spectroscopy showed that the films were nearly stoichiometric CuInS2. X-ray diffraction pattern confirmed the crystalline state of the CuInS2 films. Film microstructure and orientations were studied in function of the deposition parameters such as substrate (fused SiO2, Si(100) substrate, or In2O3 buffer layers) and carrier gas flow rate. Films deposited on fused SiO2 or Si(100) substrates exhibited the uncommon [220] orientation whereby the degree of orientation depended on the carrier-gas flow rate. Films deposited on In2O3 buffer layers were highly [112]-oriented. Carrier-gas flow significantly influenced the film microstructure. Films deposited at the lowest flow rate exhibited dendritic microstructures and were visually rough and black, whereas films deposited at the highest flow rates were visually the most uniform and reflective, and were blue with a microstructure consisting of non-faceted, elongated grains. Films deposited at intermediate flow rate exhibited dense, columnar growth and faceted crystalline features.
- RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4ANSWER 21 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN1998:536748 CAPLUS
- DN
- Spray chemical vapor deposition of CuInS2 thin films for application in TI

solar cell devices

- AU Hollingsworth, Jennifer A.; Buhro, William E.; Hepp, Aloysius F.; Jenkins, Philip P.; Stan, Mark A.
- CS Dept. of Chemistry, Washington University, St. Louis, MO, 63130, USA
- SO Materials Research Society Symposium Proceedings (1998), 495 (Chemical Aspects of Electronic Ceramics Processing), 171-176 CODEN: MRSPDH; ISSN: 0272-9172
- PB Materials Research Society
- DT Journal
- LA English
- AB Chalcopyrite CuInS2 is a direct band gap semiconductor (1.5 eV) that has potential applications in photovoltaic thin film and photoelectrochem. devices. The authors have successfully employed spray CVD using the previously known, single-source, metalorg. precursor, (Ph3P)2CuIn(SEt)4, to deposit CuInS2 thin films. Stoichiometric, polycryst. films were deposited onto fused SiO2 over a range of temps. (300-400°).

Morphol. was observed to vary with temperature: spheroidal features were obtained

at lower temps. and angular features at 400°. At even higher temps. (500°), a Cu-deficient phase, CuIn5S8, was obtained as a single phase. The CuInS2 films have a direct band gap of .apprx.1.4 eV.

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1993:159854 CAPLUS
- DN 118:159854
- TI Synthesis of mixed copper-indium chalcogenolates. Single-source precursors for the photovoltaic materials CuInQ2 (Q = S, Se)
- AU Hirpo, Wakgari; Dhingra, Sandeep; Sutorik, Anthony C.; Kanatzidis, Mercouri G.
- CS Dep. Chem., Michigan State Univ., East Lansing, MI, 48824, USA
- SO Journal of the American Chemical Society (1993), 115(4), 1597-9 CODEN: JACSAT; ISSN: 0002-7863
- DT Journal
- LA English
- The mol. precursor compds. (Ph3P)2CuIn(QR)4 (1; Q = S, R = Et; Q = Se, R = Et; Q = S, R = isobutyl) for the ternary semiconductor photovoltaic materials CuInQ2 (Q = S, Se) were prepared Mol. structures of 1 show heterobimetallic compds. with 2 thiolates/selenolates bridging Cu and In atoms forming a CuIn(QR)2 core. The tetrahedral Cu and In coordination spheres are completed by terminal R3P and QR- ligands, resp. Crystal data for 1: space group C2/c, R/Rw = 0.037/0.043; P.hivin.1, R/Rw = 0.038/0.031; P.hivin.1, R = 0.12, resp. Vacuum thermolysis of (Ph3P)2CuIn(QR)4 at 400° gives single phase crystalline CuInQ2.
- L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1991:74060 CAPLUS
- DN 114:74060
- TI Synthesis, reactions and characterization of bi- and ter-metallic alkoxides of copper(II) with aluminum(III), zirconium(IV), niobium(V) and tantalum(V)
- AU Chhipa, R. C.; Singh, A.; Mehrotra, R. C.
- CS Dep. Chem., Univ. Rajasthan, Jaipur, 302004, India
- SO Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1990), 20(8), 989-99 CODEN: SRIMCN; ISSN: 0094-5714
- DT Journal
- LA English
- AB [(Me3CO) 4A1]Cu[M(OCHMe2)x] (M = A1, x = 4; M = Nb or Ta, x = 6), [(Me3O) 4A1]Cu[Zr2(OCHMe2)9], [(Me2CHO) 4A1]Cu[Ta(OCHMe2)6] (I) and [(Me2CHO) 6Nb]Cu[Ta(OCHMe2)6 (II) were synthesized by the equimolar

interaction of the appropriate chlorobimetallic alkoxide of Cu(II) with a suitable potassium alkoxometallate. Methanolysis of II produced [(MeO)6Nb]Cu[Ta(OMe)6]. The alcoholysis reactions of I with PrOH, MeOH, or Me3COH gave rise to [(RO)4Al]Cu[Ta(OR)6] (R = Pr, Me), [AlCuTa(OMe)6(OCHMe2)4], or [(Me3CO)3(Me2CHO)Al]Cu[Ta(OCHMe2)2(OCMe3)4]. All these new derivs. were characterized by elemental analyses, IR, electronic spectral studies, and mol. weight as well as magnetic susceptibility measurements.

- L4 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1990:110706 CAPLUS
- DN 112:110706
- TI New chloro, alkoxo and allied bimetallic derivatives of copper(II) and aluminum(III)
- AU Chhipa, R. C.; Singh, A.; Mehrotra, R. C.
- CS Dep. Chem., Univ. Rajasthan, Jaipur, 302 004, India
- SO Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical & Analytical (1989), 28A(5), 396-9
 CODEN: IJCADU; ISSN: 0376-4710
- DT Journal
- LA English
- AB ClCu{Al(OCHMe2)4} was prepared by the interaction of CuCl2 and K{Al(OCHMe2)4} in equimolar proportions. ((Me2CHO)Cu{Al(CHMe2)4}) (I) was prepared by the reaction of CuCl2, KOCHMe2 and K{Al(OCHMe2)4} in 1:1:1 molar ratio. The interaction of chloro bimetallic alkoxides with KOR gives (RO)Cu{Al(OCHMe2)4}. I undergoes alc. interchange reactions, the facile nature of which is governed by the length and branching of the hydrocarbon chains of alcs. e.g. MeOH, EtOH, PrOH, sec-BuOH, tert-BuOH. The reaction with iso-BuOH gives only the mixed bimetallic alkoxides. The products were characterized by elemental analyses, mol. wts., IR, electronic spectral and magnetic susceptibility measurements.
- L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1988:230854 CAPLUS
- DN 108:230854
- TI Chloride and alkoxide alkoxometallates and termetallic isopropoxides of copper(II)
- AU Dubey, Raj K.; Singh, Anirudh; Mehrotra, Ram C.
- CS Dep. Chem., Univ. Rajasthan, Jaipur, 302004, India
- SO Journal of Organometallic Chemistry (1988), 341(1-3), 569-74 CODEN: JORCAI; ISSN: 0022-328X
- DT Journal
- LA English
- AB [CuClL] [L = Zr2(OCHMe2)9, Ta(OCHMe2)6] were prepared and characterized by IR spectra, and are key precursors in the preparation of [CuLL1] [HL1 = MeOH, Me2CHOH, BuOH, EtMeCHOH, Me3COH] and [CuL{Zr2(OCHMe2)9)] [HL = HAl(OCHMe2)4, HGa(OCHMe2)4, HTa(OCHMe2)6].
- L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1981:609778 CAPLUS
- DN 95:209778
- TI Electronic structure of simple and bimetallic alkoxides of later '3d' transition elements
- AU Mehrotra, R. C.
- CS Chem. Lab., Univ. Rajasthan, Jaipur, India
- SO Coordination Chemistry (1981), Volume Date 1980, 21, 113-25 CODEN: CCHEDK; ISSN: 0069-9845
- DT Journal
- LA English
- AB The alkoxy group (-OR) functions is a bridging ligand between similar and different metal atoms giving rise to coordination oligomers and bimetallic alkoxides. The syntheses of a large number of simple alkoxides of Cr(III &

IV), Mn(II), Fe(II & III), Co(II), Ni(II) and Cu(II) were described. Most of these are non-volatile and insol. in organic solvents, except (t-BuO)4C and alkoxides or Fe(III), Fe(OR)3, in general. These polymeric new alkoxides of later '3d' metals differ from the alkoxides of earlier transition and main group elements in the comparatively much lesser lability of their alkoxy groups in general. The sharp differences in the alcoholysis reactions of these alkoxides with ramification of the alkyl group were correlated with the changes in the stereochem. of the alkoxide derivs. as revealed by physico-chemical studies. A large number of monomeric volatile bimetallic isopropoxides of the above elements with Al, having the general formula M[Al(Oi-Pr)4]n were described for the 1st time. Structures of all these derivs. were suggested on the basis of spectroscopic (visible, UV, IR and ESR) and magneto-chemical studies, with tetraalkoxy aluminate moieties functioning as univalent bidentate and in some cases as tridentate ligands.

- L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1979:412926 CAPLUS
- DN 91:12926
- TI Volatile double isopropoxides of later transition metals with aluminum
- AU Singh, J. V.; Jain, N. C.; Mehrotra, R. C.
- CS Chem. Lab., Univ. Delhi, Delhi, 110007, India
- SO Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1979), 9(1), 79-88
 CODEN: SRIMCN; ISSN: 0094-5714
- DT Journal
- LA English
- AB The liquid monomeric complexes M[Al(OPr-iso)4]n (M = Cr, Fe, n = 3; M = Co, Cu, Mn, Ni, n = 2) were prepared and characterized by chemical anal., mol.-weight
- detns., solubility in organic solvents, and IR spectra. The [Al(OPr-iso)4]-ion acts as a bidentate ligand in these complexes.
- L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1979:161457 CAPLUS
- DN 90:161457
- TI Ligand field spectroscopic studies of transition metal-aluminum tetraalkoxides
- AU Stumpp, Eberhard; Hillebrand, Uwe
- CS Anorg.-Chem. Inst., Tech. Univ. Clausthal, Clausthal-Zellerfeld, Fed. Rep. Ger.
- SO Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1979), 34B(2), 262-5 CODEN: ZNBAD2; ISSN: 0340-5087
- DT Journal
- LA German
- AB The preparation and electronic spectral properties of M[Al(OR)4]2 (M = Co, Ni, Cu; R = Me, Et, Pr, Bu) are described. The spectral data are used in conjunction with ligand-field theory in deducing the structures of the compds. The spectrum of green Ni[Al(OR)4]2 is interpreted as a Ni(OR)6 octahedron sharing faces with 2 Al(OR)4 tetrahedrons. Co2+ and Cu2+ are in a distorted octahedral coordination. The alkoxide ligands are fitted into the spectrochem, and the nephelauxetic series. They are close to H2O in these series.